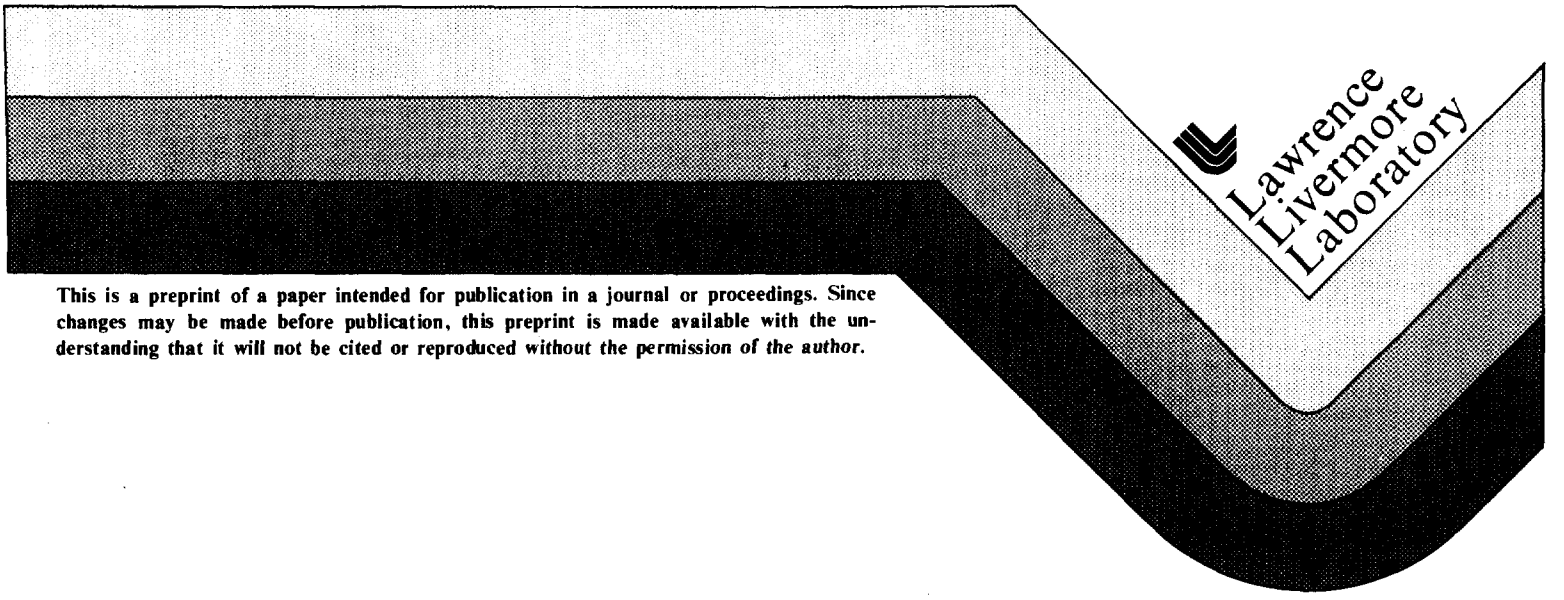
UCRL-82236
PREPRINT

A REPOSITORY POST-SEALING RISK ANALYSIS USING MACRO

A. M. Kaufman
L. L. Edwards
W. J. O'Connell

This paper was prepared for submittal to:
Waste Management '80 Symposium
March 10-14, 1980
Tucson, Arizona

February 14, 1980



ABSTRACT

A REPOSITORY POST-SEALING RISK ANALYSIS USING MACRO

by

A. M. Kaufman, L. L. Edwards, and W. J. O'Connell

MACRO, a code to propagate probability distributions through a set of linked models, is currently under development at Lawrence Livermore Laboratory. An early version of this code, MACRO1, has been used to assess post-sealing dose to man for simple repository and site models based on actual site data.

A REPOSITORY POST-SEALING RISK ANALYSIS USING MACRO*

A. M. Kaufman, L. L. Edwards, W. J. O'Connell
Lawrence Livermore Laboratory

INTRODUCTION

The assessment of dose to man from a nuclear waste repository is among a class of problems in which uncertainty of information can have a major impact. A risk analysis of a repository plus site is therefore necessary in order to determine, first of all, the feasibility of a chosen site, and secondly, the degree of conservatism required in various necessary engineering decisions. Part of the process of analysis is the determination of the probability of exceeding a dose criterion. This probability is an expression of the risk presented by the waste isolation system.

At Lawrence Livermore Laboratory, we have been developing a tool with which to assess the impact of parameter uncertainty on systems such as a waste isolation system. The tool is a code called MACRO. A test version of this tool called MACRO1[1], has already been implemented to do a post-sealing risk analysis and is running at LLL. MACRO1 has been run using actual geophysical data and its uncertainty to analyze what we call a "mock" site.

In the "mock siting exercise", real geophysical data were used in order to (1) determine the extent that a risk analysis using the relatively simple models in MACRO1 was possible, and (2) test the methods employed in such an analysis. The feasibility of the site and repository was not the primary objective.

An important conclusion to be drawn from our analysis is that correlations of input parameters have an important influence on the conclusions to be drawn from the analysis. The net effect of correlations is often a reduction of uncertainty in system performance. In hydrological transport modeling, important in the waste management problem, a correlation exists between

*This work was supported by the United States Nuclear Regulatory Commission under a Memorandum of Understanding with the United States Department of Energy.

porosity and permeability. Since MACRO1 was able to handle correlations in only a limited way, a thorough exploration of this issue was not pursued.

As a result of our work, we feel that simple models of a system with large uncertainties offer a reasonable approach in a risk assessment. MACRO1 as a tool, limited though it is, seemed to do a creditable job of analysis, especially when compared to results of more time consuming Monte Carlo runs of a code[2] using similar models.

MACRO

There is a large class of systems in which uncertainty plays an important, if not dominant, role. The waste isolation system involving deep geologic disposal belongs to this class. Many methods have been devised to deal with uncertainty. Among them are fault trees, Monte Carlo, moment expansions, latin hypercube, etc.

The analysis of any one system involves a tremendous programming effort. First, models which describe the performance of the subsystems must be built, and second, various uncertainty propagation algorithms must be implemented. The second step is highly repetitive and involves great duplication of effort for each system to be analyzed.

MACRO provides a much quicker avenue towards an uncertainty analysis by requiring only that the analyst program the routines which describe the system. A program user language is used to guide the uncertainty analysis itself. In the ultimate version of the code, the analyst will have choice of methodology for uncertainty propagation as well.

The current version of MACRO, called MACRO1, is now running at LLL, and contains a simple uncertainty propagation methodology which we shall briefly describe.

Finite Probability Distributions

For any variable, x, let $x_1, x_2, \ldots, x_n$ be representative values for a collection of disjoint neighborhoods. For example, mid-points of a collection of half-open intervals on the real

line for a scalar x. We express our state of knowledge about the variable x by assignment of probabilities, $p_1, p_2, \ldots, p_n$, the probability that x is in the neighborhood designated by x_n. This assignment of probabilities may be done directly or as a finite approximation to some given probability density function.

The collection of doublets

$$\{\langle x_1, p_1\rangle, \langle x_2, p_2\rangle, \ldots, \langle x_n, p_n\rangle\}$$

is referred to as a finite probability distribution (FPD) representing our state of knowledge about the variable x. We require that $p_1 + p_2 + \ldots + p_n = 1$.

For scalar variables, the FPD may be thought of as a histogram; however, the neighborhoods need not be uniform.

Probabilistic Arithmetic

Suppose x and y are independent, uncertain variables and suppose our state of knowledge with respect to x and y are expressed by the FPD's (histograms)

$$x = \{\langle x_i, P_i\rangle;\ i=1,2,\ldots,\overline{i}\}$$

$$y = \{\langle y_j, Q_j\rangle;\ j=1,2,\ldots,\overline{j}\}$$

Let $\otimes$ stand for a deterministic combining of "inputs" x and y to an output variable, i.e.,

$$Z = x \otimes y$$

where $\otimes$ may be simple arithmetic or $\otimes$ may, in fact, be a "physics model".

Then, following the methodology of Kaplan[3], we compute the output FPD by

$$\text{First:} \quad \{\langle Z_{ij}, R_{ij}\rangle = \{\langle x_i \otimes y_j, P_i Q_j\rangle \left| \begin{array}{l} i=1,2,\ldots,\overline{i} \\ \\ j=1,2,\ldots,\overline{j} \end{array} \right.\}$$

Second: Apply the condensation operation to a previously discretized output space to obtain

$$\{\langle Z_k, S_k\rangle;\ k=\underline{k},\underline{k}+1,\ldots,\overline{k}-1,\overline{k},\ \sum_k S_k=1\}$$

where

$$S_k = \sum_{\{i,j;Z_{ij}\,\epsilon\, N(Z_k)\}} P_i Q_j$$

and

$$\underline{k} = \text{minimum}\ \ k;S_k \neq 0$$

$$\overline{k} = \text{maximum}\ \ k;S_k \neq 0\ .$$

Third: If desired, discard the low probability tails by truncation followed by renormalization.

If x and y are dependent, they are represented by a joint FPD, which is R_{ij}.

The extension to more than two variables is straightforward; however, to gain computing speed, we "factor models" whenever possible and apply the condensation and truncation operations at intermediate steps.

The computing speed of MACRO1 is greatly enhanced by using the condensation operation at intermediate steps of "factored models". The concept of factorization can be most readily described by a simple example.

Suppose our "model" is

$$w = xyz$$

and further suppose that each of x, y, and z are FPD's with 10^2 entries of non-zero probability. The straightforward 3-deep do-loops of the methodology would then require 10^6 multiplications.

Suppose that we "factor" the model to

$$u = xy$$

$$w = uz$$

mathematically equivalent by the associative law. In this case, $u = xy$ requires 10^4 multiplications and if u "condenses" to any number of neighborhoods less than 10^4-10^2 we gain computationally. If, for example, u condenses to 10^2 neighborhoods, $w = uz$ requires 10^4 multiplications. But then, $w = uz = (xy)z$ requires a total of 2×10^4, considerably less than 10^6.

One should note that if inputs are mutually dependent, or if multiple outputs are generated, extreme care must be taken in the factorization. It may not be possible to readily or accurately factor some models. Another example is in order.

Suppose we wish to solve a one-dimensional hydrology and transport model. We are given

ΔH = head difference

L = length of flow path

K = hydraulic conductivity

n = effective porosity

and the physics equations for the D'Arcy velocity q, the water particle velocity v, and the transport time t:

$$t = \frac{L}{v}$$

where

$$v = \frac{q}{n}$$

and

$$q = \frac{-k\Delta H}{L}$$

If we assume that ΔH, L, K, and n are all independent, we might compute in a "factored" mode

$$G = \frac{\Delta H}{L}$$

$$q = -GK$$

$$v = q/n$$

$$t = L/v$$

which erroneously neglects the fact that the L in the last factor is identical with (therefore dependent on) the L in the first factor.

If we now write

$$k = K/n$$

$$y = -\Delta H/x$$

$$t = L^2/y$$

the deterministic result is the same and we use the probability over L only once.

Suppose that k and n are closely correlated, then the computation of x in the above sequence can be readily accommodated and this factorization is acceptable. If, however, ΔH, K, and n were somehow correlated (a joint FPD), the above model would have to be factored differently or the basic methodology altered.

The primary point is, factorization can gain computing speed, however, one must factor consistent with the "probabilistic arithmetic methodology" and correlation of variables rather than with physics notions.

MOCK SITE ANALYSIS

A mock site study[4] was done to develop and extend our site assessment methodology by exercising it on a real geological site. A region was selected with layered sedimentary geology and with extensive data already available from a mineral and groundwater exploration program. A nominal site was selected in a low-permeability shale layer below the main regional aquifer (see Fig. 1).

Geosphere Transport Model

At the site, a downward hydraulic gradient carries any leached waste away from the aquifer; the waste can reach surface

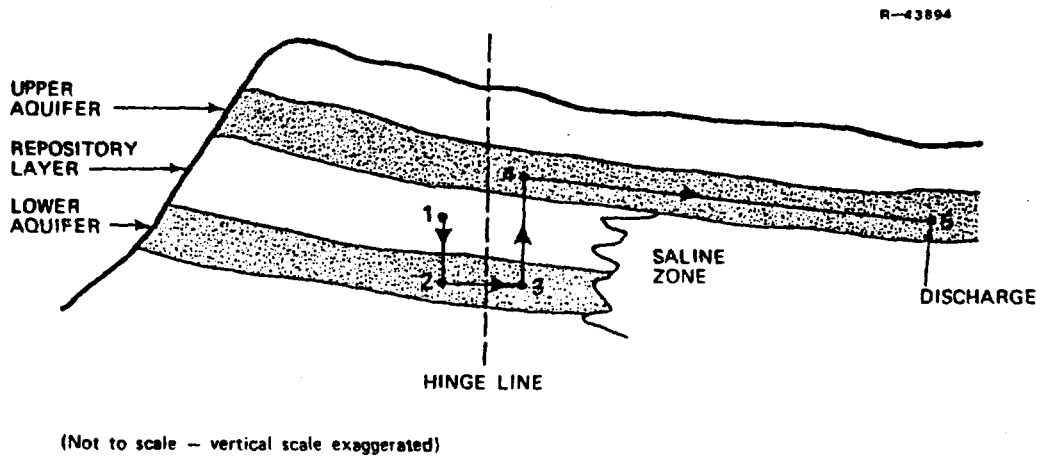


Fig. 1. Regional cross section and basic flow path model.

water only after moving along the semi-isolated lower aquifer, back to the upper aquifer, and then to a discharge into a stream near the center of the basin. The aquifers' flow lines are roughly parallel in the area of interest, so the two-dimensional section of Fig. 1 is reasonable. The flow is further simplified to a series of four one-dimensional flow paths in the model illustrated in Fig. 1. This is only a coarse approximation in the zone 3-4; the return flow to the upper aquifer occurs along the entire area from the "hinge line" to the end of the lower aquifer, with a varying vertical head difference. An average location and head drop were selected for the 1-D segmental model. This simple model is useful for getting a first idea of the future performance, its uncertainty, and its controlling parameters. (Other flow patterns and accident scenarios could be modeled in a similar way; we limit the following to this first flow scenario.)

Table I gives the geosphere transport model parameters and their uncertainties, based on interpreting and averaging the field data over the volumes that we model as one-dimensional flow paths. Some uncertainties are rather high due to sparse data, spatial variability, and difficulty of measuring transport parameters.

TABLE I. Parameter Values and Uncertainties

Pipe	Length (L),m	Head difference (ΔH), m, or hydraulic gradient (i)	Effective porosity (n)	Hydraulic conductivity (K), m/y	Retardation factor (R_d) for fission products
1-2	59.5 (0.14)	42.9 (0.10)	0.001 (0.5)	0.027 (0.65)	100. (1.0)
2-3	4835 (0.057)	0.0015 (0.22)	0.015 (0.5)	754 (0.18)	7.8 (0.4)
3-4	119 (0.14)	16. (0.044)	0.001 (0.5)	0.12 (0.50)	5. (0.3)
4-5	15000 (0.05)	0.015 (0.058)	0.012 (0.5)	289 (0.44)	65. (0.9)

NOTES: Figures in brackets refer to $\sigma(\log_{10} t)$. Estimates are made assuming that uncertainty distributions are lognormal and that parameters are independent.

The performance of the geosphere transport is represented by the first two moments of the transport Green's function, t and S^2 (mean time of exit and pulse width squared), which can be calculated algebraically. For a single path

$$t = \frac{L^2 n R_d}{K \Delta H}$$

$$S^2 = 2\alpha L^3 \left(\frac{n R_d}{K \Delta H}\right)^2$$

where L is the path length and ΔH is the head drop. The outputs S and t are obviously correlated.

The overall geosphere transport Green's function's moments t_g and S_g are computed from those of the individual paths in the series:

$$t_g = \sum_i t_i \qquad S_g^2 = \sum_i S_i^2$$

We compute the values and FPD for the correlated pair for a single group of nuclides with a common R_d. We have not looked at the radioactivity flux from all nuclides together; the R_d's of the various nuclide groups are expected to be strongly correlated.

Waste Dissolution Model

We assume a rectangular dissolution function: starting at time D_o and continuing at a constant rate I_o/S_d for a time duration S_d (where I_o is the initial inventory of waste).

Table II gives the parameters. We assume that the start time (due to waste age at closure plus canister corrosion time) is fully correlated to the duration time.

TABLE II. Waste dissolution model parameters.

Parameter	Method of Calculation	Value and Uncertainty
Starting Time D_o	$D_o = 32 + y$	For y: 60 (0.23)
Pulse Duration S_d	$S_d = 2000 \times (y/60)^{1.3}$	2000 (0.30)

Biosphere Hazard Model

MACRO uses the resources of the BIODOSE[5] program for the biosphere effects, going from the influx of radioactivity through ecologic compartments to human dose. We assume that the influx changes only slowly with time so that there is roughly a steady state in the biosphere compartments (including the buildup of some nuclides in irrigated soil). The resulting dose hazards are stored as tables H(t). We do not consider uncertainty here.

Fig. 2 shows the hazard functions for our three nuclide groups, for an assumed Columbia-like river basin.

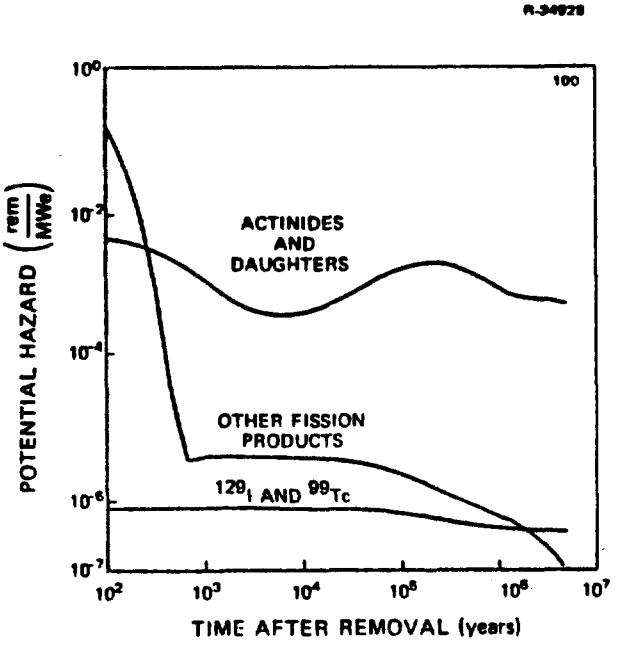


Fig. 2. The potential hazard of spent fuel measured as a 50 year whole-body-equivalent dose to an individual with an average diet and in the most disadvantageous locality.

Combination of Models

The following three models are combined to get the dose and its FPD for a nuclide group:

- the dissolution model, with one uncertain parameter S_d (and one dependent parameter D_o);
- the geosphere transport model with its two correlated uncertain parameters t_g and S_g;
- the biosphere hazard model with its unit hazard tables H(t), without uncertainty.

The method is as follows, for each combination of the three input uncertain variables:

1. Model the overall transport Green's function J(t) using a one-path functional form with the moments t_g and S_g^2.

2. Compute the radioactivity flux F(t) by convoluting J(t) with the dissolution function.

3. Compute the peak dose, by finding the time t_p of peak radioactivity flux. Then

$$\text{Peak Dose} = F(t_p) \times H(t_p)$$

Special cases:

(i) If $S_d \ll S_g$, then neglect S_d and use the Green's function multiplied by I_o as the convoluted function.

(ii) If $S_d \gg S_g$, then neglect S_g and use the dissolution function as the convoluted function (but shifted in time by the transport time t_g). Then

$$\text{Peak Dose} = \frac{I_o}{S_d} \times \underset{t}{\text{Max}} \left[H(t) \middle| t_g + D_o \leq t \leq t_g + D_o + S_d \right]$$

The above combination model was coded as a problem-specific subroutine with three scalar input variables. MACRO's general procedures took care of looping over the three uncertain input variables and sorting the results and their probabilities.

Application

The combination of the site data and uncertainties, the physics models, and MACRO's uncertainty propagation procedure is illustrated now for the mock site and for our nuclide group II, the positive-ion fission products which have a moderate retardation. Fig. 3 shows the FPD for the time of peak dose; the variability is predominantly that of the geosphere transport time t_p. Fig. 4 shows the FPD for the peak dose (50-year dose in rem to an individual of average lifestyle, living in the most disadvantageous location). The expected dose is about 10^{-9} rem per 50 years, but there is a finite probability of a peak dose as high as 5×10^{-6} rem per 50 years. (The figure's units are dose per MWe-yr equivalent of spent fuel; multiply by 10^6 MWe-yr for a full-scale waste repository.) Note that the uncertainty is that

due to the waste form and geosphere. The result and uncertainty might be considered to be for waste flux in curies/year; a conversion to dose effects using one surface water system was done to account for the different impact per curie of different nuclides, and to bring the consequence measure closer to our actual concerns.

As expected, the mean time and pulse width in geosphere transport are highly correlated; probability contours for this output correlation are shown in Fig. 5. The peak dose is also highly correlated to the time of the peak dose; this is illustrated in Fig. 6. The peak dose decreases sharply with time of peak, first, because of the rapidly declining hazard function (see Fig. 2), and further because the peak dose is inversely correlated to the transport pulse width which increases as the peak time increases.

Conclusions

Looking at Figs. 4 and 6, we see that the higher dose values in the distribution make the mock site unacceptable. (Although specific quantitative dose-risk criteria are not yet established, we feel that a better performance is reasonably achievable at many other sites.) In Fig. 6, if by better site selection we can move the median transport time for group II nuclides up by a factor of thirty, then the lowest probability contour used will lie entirely below 10^{-8} rem per 50 years per MWe-yr (0.2 millirem per year from a full repository of 10^{6} MWe-yr of spent fuel), even with almost an order of magnitude uncertainty as shown in Fig. 4. Such a dramatic improvement is not usually obtainable by a shift of the median value. A reduction of the uncertainty in the transport time (which could be achieved by better site and regional investigation), without a shift in its median, would also dramatically reduce the risk of high dose effects.

MACRO has proved to be a functioning and flexible tool for nuclear waste repository long-term performance risk analysis. Despite the extreme simplicity of the physics models used in the application, we have gained insight into the parameters and the extent of impact of the uncertainties. Parameter correlations are the next area we plan to address.

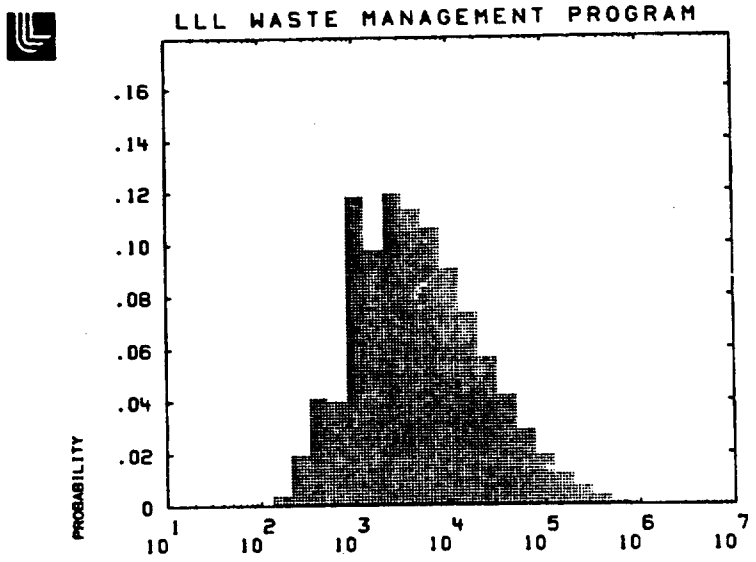


Fig. 3. Finite probability distribution (FPD) histogram for the time of peak dose, for nuclide group II (fission products).

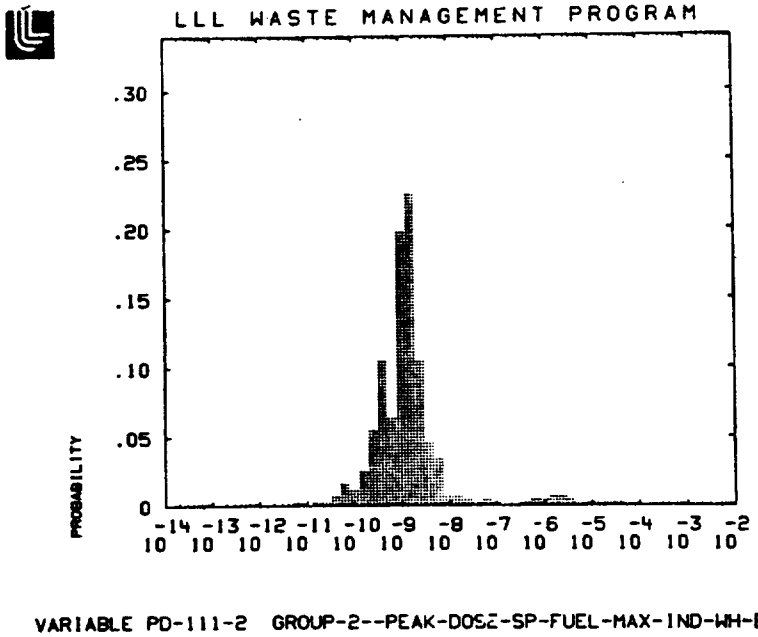


Fig. 4. FPD histogram for peak dose to an individual, in rem per 50 years, for nuclide group II.

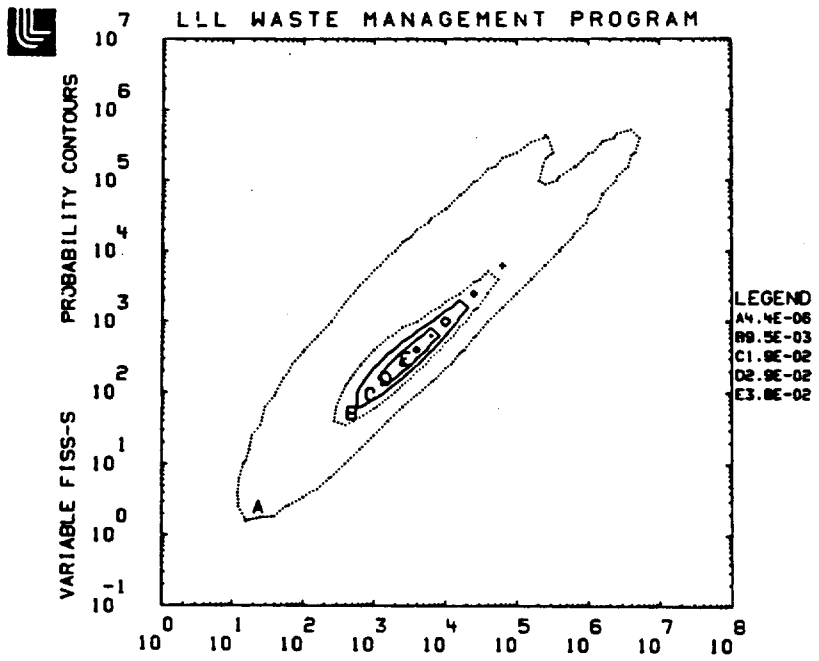


Fig. 5. Correlated probability density for pulse mean arrival time and pulse width in time, in years, for nuclide group II.

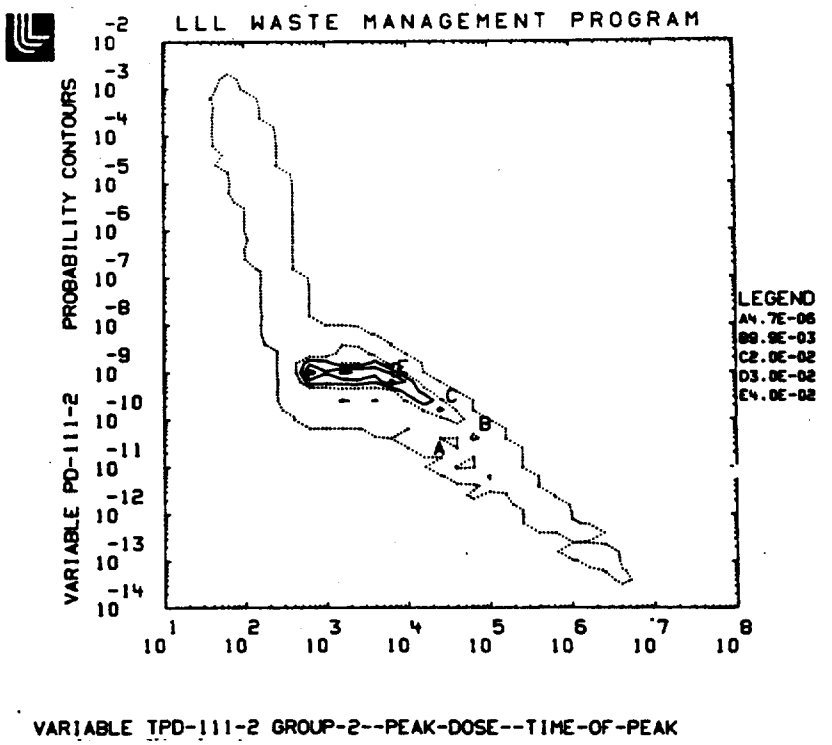


Fig. 6. Correlated probability density for mean arrival time, in years, and peak dose, in rem per 50 years, for nuclide group II.

REFERENCES

1. L. L. Edwards, MACRO1: A Systems Uncertainty/Sensitivity Analysis Methodology, Lawrence Livermore Laboratory, UCRL-52736, in press.

2. M. Giuffre, and M. Kaplan, An Example of Monte Carlo Analysis Applied to Repository Siting, The Analytic Sciences Corp., Reading, MA, TR-1797-2, August, 1979.

3. Kaplan & Associates, Inc., Notes on the LLL/NRC Waste Disposal Study II - Probabilistic Arithmetic, UCRL-13998-2, May, 1978.

4. W. J. O'Connell, Mock Site "A" Assessment, Lawrence Livermore Laboratory, UCRL-52718, in press.

5. B. Ross, C. M. Koplik, M. S. Giuffre, S. P. Hodgin, J. J. Duffy, NUTRAN: A Computer Model of Long-Term Hazards from Waste Repositories, The Analytic Sciences Corp., Reading, MA, UCRL-15150, December, 1979.